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*Published in:*  
Chemical Physics Letters

*DOI:*  
[10.1016/j.cplett.2004.07.096](https://doi.org/10.1016/j.cplett.2004.07.096)

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*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2004

[Link to publication in University of Groningen/UMCG research database](#)

### *Citation for published version (APA):*

van Faassen, M., Jensen, L., Berger, J. A., & de Boeij, P. L. (2004). Size-scaling of the polarizability of tubular fullerenes investigated with time-dependent (current)-density-functional theory. *Chemical Physics Letters*, 395(4-6), 274 - 278. <https://doi.org/10.1016/j.cplett.2004.07.096>

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# Size-scaling of the polarizability of tubular fullerenes investigated with time-dependent (current)-density-functional theory

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Received 19 July 2004; in final form 19 July 2004

Available online 20 August 2004

## Abstract

We present a study of the static polarizability for the tubular fullerenes  $C_{60+i \times 10}$ , where  $i = 0-5$ , and the closely related [5,5] carbon nanotube, using time-dependent (current)-density-functional theory. Comparing the results obtained within the conventional adiabatic local-density approximation with those obtained using the Vignale–Kohn current-dependent exchange-correlation functional it is found that the extra long-range exchange-correlation effects described by the current-density functional are important to consider, especially for the longest fullerenes. For all systems studied the current-density functional results are in good agreement with experiment, and the agreement with available ab initio self-consistent-field results and results from a point–dipole interaction model is much better than when using the adiabatic local-density functional.

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The dipole–dipole polarizability of an atomic cluster is next to being determined by its chemical composition also strongly influenced by the size and shape of the cluster. Characterizing these clusters by evaluating the dependence of the polarizability on the cluster geometry has therefore been an important research area [1–10]. The reason for the strong dependence is easily understood using an interacting point–dipole model of the cluster. As the self-consistent local fields acting upon the polarizable atoms will depend strongly on the arrangement of the atoms, so will the resulting induced dipole moments, which constitute the total response of the system. By adding more and more atoms to the cluster the effective polarizability per atom, which links the mean induced dipole moment per atom to the average local field, should converge towards a bulk value. This value is related to the experimental

susceptibility of the bulk material via the famous Lorentz–Lorenz relation [10]. Typical systems studied are alkali-metal clusters [1–3] and semi-conductor clusters [4–6]. Another class is formed by the all-carbon clusters, which have attracted a lot of attention since their discovery, such as the fullerenes [11] and the carbon nanotubes [12]. In this paper, we will investigate the size dependence of the polarizability for the tubular fullerenes  $C_{60+i \times 10}$ , where  $i = 0-5$ . These tubular fullerenes can be considered to be capped [5,5] carbon nanotubes as is illustrated in Fig. 1.

We will use time-dependent (current)-density-functional theory (TD-(C)DFT) in this study. It is well established that conventional density-functional response or finite-field calculations that use the adiabatic local-density approximation (ALDA) for the induced exchange-correlation effects tend to overestimate the polarizability and hyperpolarizability of conjugated polymers, especially for the longer oligomer chains [13,14]. The local approximation and also more advanced generalized gradient approximations (GGA) are unable to describe the highly nonlocal exchange and correlation

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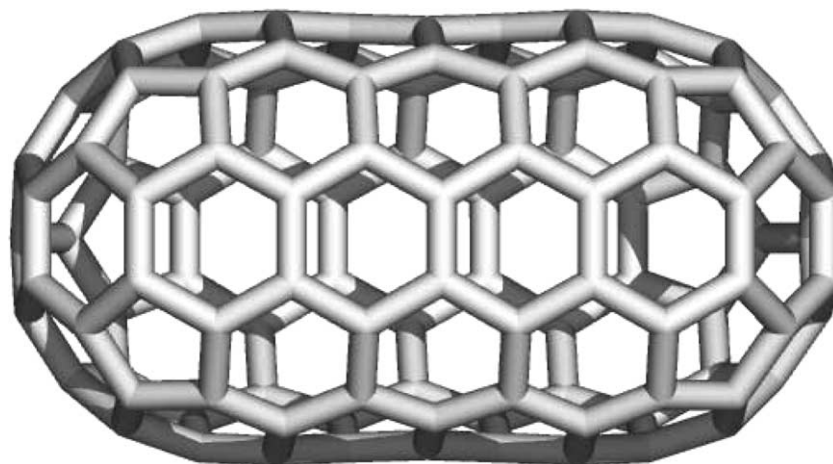


Fig. 1. Structure of the  $C_{110}$  tubular fullerene.

effects found in these systems [13,14]. One way to overcome these shortcomings is to employ optimized effective potentials [15–17] or approximations to this potential [18,19]. We have found in our previous works [20,21], a successful alternative approach towards the solution of this problem by using TD-CDFT. In this approach the long-range exchange-correlation effects are described within a local-current-density approximation, for which we use the Vignale–Kohn (VK) functional [22]. With this method, the results obtained for the prototype conjugated polymers like polyacetylene are in excellent agreement with high-level *ab initio* quantum chemical methods. The reason for choosing the tubular family of fullerenes in this study is that we can determine to what extent the highly nonlocal exchange-correlation effects are important for these fullerenes. If long-range effects are indeed important, it is expected from the studies of the conjugated polymers that these contributions become more important with increasing tube length. The aim is both to investigate the size dependence of the polarizability for larger fullerenes and to assess the quality of the density- and current-density-dependent approximations for treating these all-carbon molecules within DFT.

For the smallest fullerene,  $C_{60}$ , a reasonably accurate experimental value and some theoretical calculations are available for the static polarizability. In comparing the various results it is found that the conventional DFT result of 543.8 a.u. reported in literature [23] is slightly higher than the *ab initio* self-consistent-field (SCF) result of 506.7 a.u. [24] and the result from the point-dipole interaction (PDI) model of 522.9 a.u. [25]. All these values are in agreement with the experimental value of  $516.2 \pm 54$  a.u. [7]. Other studies also indicate that conventional DFT predicts a polarizability for  $C_{60}$  that is larger than obtained with *ab initio* methods [26]. It is therefore interesting to investigate if some of the differences between the conventional DFT results

and *ab initio* SCF results for the  $C_{60}$  molecule are caused by highly nonlocal exchange-correlation effects.

We performed the TD-(C)DFT calculations within the linear response formulation. The calculations of the polarizability were done using the ALDA and the VK approximation for exchange-correlation functionals, with the use of a modified version of the Amsterdam Density Functional (ADF) program package [27,28]. For the ALDA calculations we used a ground-state description obtained within the statistical averaging of (model) orbital potentials method (SAOP) [29], which is a shape-corrected potential constructed for the calculation of molecular response properties. The SAOP ground-state potential usually gives superior results for the (hyper)polarizability compared with LDA and GGA potentials [29]. The VK response calculations, on the other hand, were performed using the standard LDA description of the ground state, as this description is compatible with the VK functional. The structures of the fullerenes  $C_{60}$ – $C_{100}$  were taken from [30] and the structure of  $C_{110}$  from [31]. The structure of  $C_{100}$  was relaxed in order to obtain the correct symmetry. For the model PDI calculations, the structures used were optimized at the PM3 level and taken from [31], which is consistent with the PDI model parametrization [32]. All structures are available from the authors upon request.

We compare our results with experimental data, with results obtained using wavefunction methods, and with results obtained using the PDI model [25,32]. Experimental results for the dipole–dipole polarizabilities of the  $C_{60}$  and  $C_{70}$  molecules have recently been obtained in the gas phase with the use of molecular beam experiments [7–9]. For  $C_{60}$  a value of  $516.2 \pm 54$  a.u. was reported for the static polarizability [7], and a value of  $533 \pm 27$  a.u. was measured for the polarizability at the frequency 0.0428 a.u. ( $\lambda = 1064$  nm) [8]. For both the static and the frequency-dependent polarizability, the experimental results are in good agreement with

recent quantum chemical calculations [23,24] and results from a frequency-dependent PDI model [25,32]. For  $C_{70}$  an experimental value of  $688 \pm 94$  a.u. was reported for the static value [9] whereas the ab initio SCF result is 605.9 a.u. [24]. Thus far there have been no DFT calculations reported for the polarizability of the fullerenes larger than  $C_{60}$ .

We first study the basis-set dependence of the results for the mean polarizability,  $\bar{\alpha} = \frac{1}{3}(2\alpha_{\perp} + \alpha_{\parallel})$  with  $\parallel$  and  $\perp$  indicating the directions along and perpendicular to the long axis of the molecule, that are obtained using the SAOP/ALDA combination of ground-state and response potentials. The basis sets used are the standard ADF basis set of double zeta plus polarization function (DZP) quality, the valence triple zeta plus polarization function (TZP) quality, and the TZP basis augmented with additional first-order field-induced polarization functions (TZP+) [33]. The TZP+ basis set is expected to give results for the polarizability which are close to the basis-set limit [33]. Attempts to go beyond the TZP+ quality induced linear dependency of the basis set, effectively reducing the accuracy of the calculations. In Table 1 we present the mean polarizability for the tubular fullerenes calculated using the SAOP/ALDA potentials and different basis sets. The results are also plotted in Fig. 2. From these results we see that the mean polarizability for each fullerene gradually increases in going from DZP to TZP+. We also see that for the larger fullerenes the difference in the polarizability obtained with TZP and TZP+ becomes smaller. From Fig. 2 we see that the size-dependence of the polarizability for the fullerenes is similar for the different basis sets used. Therefore we do not expect that basis-set effects will affect our conclusions regarding the size dependence. Since TZP+ is expected to give results close to the basis-set limit we will use this basis set in the remainder.

We can now study the results for the mean value and the two tensor components separately of the static polarizability as function of the fullerene size for the SAOP/ALDA and LDA/VK combinations. In Table 2 we present results for  $\bar{\alpha}$ ,  $\alpha_{\parallel}$ , and  $\alpha_{\perp}$  for the various

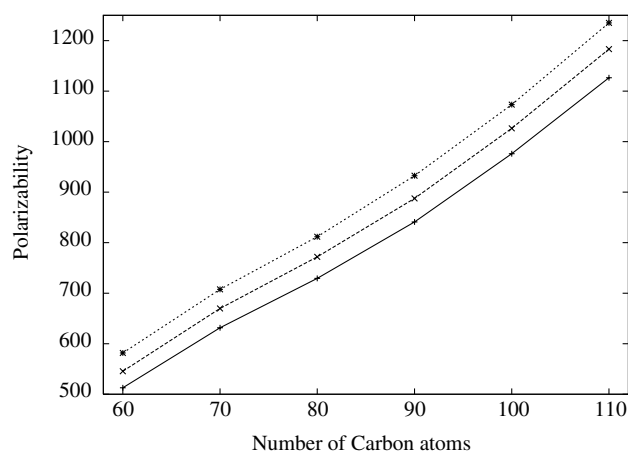


Fig. 2. Mean polarizability in a.u. of the tubular fullerenes calculated using TD-DFT with SAOP and different basis sets. (+) DZP, (×) TZP, (\*) TZP+.

fullerenes. The results for the tensor components  $\alpha_{\parallel}$  and  $\alpha_{\perp}$  have been plotted in Fig. 3 as function of the system size for the SAOP/ALDA and LDA/VK approximations. In the same figure we have also plotted the results obtained with the PDI model. From the results in Table 2 and Fig. 3 we see that for all fullerenes the polarizabilities obtained using LDA/VK are smaller than those obtained using SAOP/ALDA, and that the LDA/VK results are in close agreement with the PDI model calculations. Furthermore, we see that the differences are larger in the direction along the tube and that there is an increase in the difference as the size of the fullerenes becomes longer. For  $\alpha_{\parallel}$  we see that the difference is 10% for  $C_{60}$  whereas for  $C_{110}$  this is 22%. Especially the values for  $\alpha_{\parallel}$  obtained with SAOP/ALDA deviate more and more from the LDA/VK and the PDI results as the fullerene size increases. These results confirm that the highly nonlocal exchange-correlation effects added by the VK functional become increasingly important in the longer fullerenes. In Fig. 3 we can see that the size-dependence of the perpendicular component,  $\alpha_{\perp}$  is nearly linear, with some scattering as result of the geometries used. We see that the SAOP/ALDA results are about 65 a.u. larger than the LDA/VK results, independently from the size.

The literature LDA/ALDA value of 543.8 a.u. [23] for  $C_{60}$  was obtained in a modified TZP basis, which is in excellent agreement with the corresponding SAOP/ALDA value of 545.5 a.u. for the TZP basis. The higher SAOP/ALDA value of 581.60 a.u. obtained in the TZP+ basis is therefore mainly caused by basis set effects, which is further supported by the fact that we obtain a value of 604.47 a.u. with LDA/ALDA using the same TZP+ basis. The experimental results for the static polarizability of  $C_{60}$  is  $516 \pm 54$  a.u. [7] which is in close agreement with the SCF result of 506.7 a.u. [24], and the PDI result of 522.6 a.u. [25]. Comparing the results from

Table 1

Mean static dipole–dipole polarizability (in a.u.) of tubular fullerenes calculated using TD-DFT within the SAOP/ALDA approximation for a double-zeta plus polarization (DZP), valence triple-zeta plus polarization (TZP), and augmented TZP basis (TZP+)

Fullerene <sup>a</sup>		DZP	TZP	TZP+
$C_{60}$	D <sub>5d</sub>	512.8	545.5	581.6
$C_{70}$	D <sub>5</sub>	631.5	669.8	707.6
$C_{80}$	D <sub>5</sub>	729.3	772.0	811.7
$C_{90}$	D <sub>5h</sub>	841.1	887.6	932.5
$C_{100}$	D <sub>5</sub>	976.1	1026.4	1073.2
$C_{110}$	D <sub>5h</sub>	1126.5	1183.2	1235.0

<sup>a</sup> The Symmetry used in the calculations.

Table 2

Static dipole–dipole polarizability for tubular fullerenes (in a.u.) obtained using TD-(C)DFT within the SAOP/ALDA and LDA/VK approximations, and using the PDI model

Syst	$\alpha_{\parallel}$			$\alpha_{\perp}$			$\bar{\alpha}$		
	SAOP/ALDA	LDA/VK	PDI	SAOP/ALDA	LDA/VK	PDI	SAOP/ALDA	LDA/VK	PDI
C <sub>60</sub>	581.60	533.59	522.76	581.60	533.59	522.76	581.60	533.59	522.76
C <sub>70</sub>	758.90	683.44	668.82	681.89	620.00	591.82	707.56	641.14	617.49
C <sub>80</sub>	947.33	836.76	814.11	743.87	677.63	665.87	811.68	730.67	715.28
C <sub>90</sub>	1160.1	1005.5	977.55	818.67	752.95	735.98	932.47	837.14	816.50
C <sub>100</sub>	1420.4	1193.8	—	899.57	821.75	—	1073.2	945.76	—
C <sub>110</sub>	1698.2	1392.3	1328.8	1003.4	913.16	876.86	1235.0	1072.9	1027.5

Given are the tensor components along ( $\alpha_{\parallel}$ ) and perpendicular  $\alpha_{\perp}$  to the long axis, together with the mean value  $\bar{\alpha}$ .

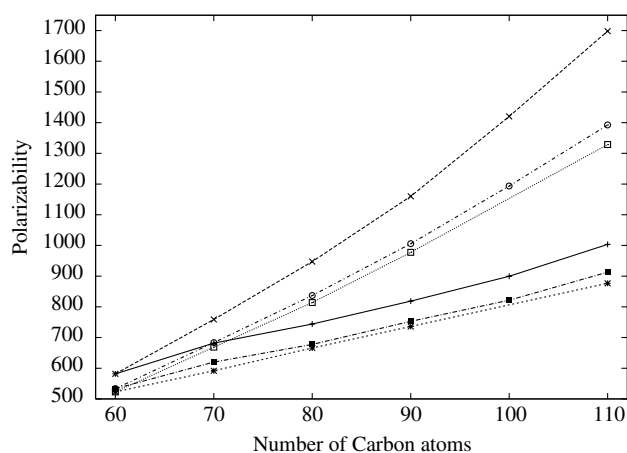


Fig. 3. The polarizability in a.u. for the fullerenes as a function of the number of carbon atoms. (\*)  $\alpha_{\perp}$  PDI, (■)  $\alpha_{\perp}$  VK, (+)  $\alpha_{\perp}$  SAOP, (□)  $\alpha_{\parallel}$  PDI, (○)  $\alpha_{\parallel}$  VK, and (×)  $\alpha_{\parallel}$  SAOP.

the present work, the value of 581.60 a.u. obtained using SAOP/ALDA and 533.6 a.u. using LDA/VK, we see that the correction due to the VK potential (−8%) brings the polarizability in close agreement with experimental, ab initio SCF and PDI results, whereas the SAOP/ALDA and LDA/ALDA results are much larger, and lay outside the experimental uncertainty range.

For C<sub>70</sub> the experimental result of  $688 \pm 94$  a.u. [9] is in fair agreement with the SCF result of 605.9 a.u. [24] and all results from the present study: 617.5 a.u. for the PDI model, 707.6 a.u. with SAOP/ALDA and 641.14 a.u. with LDA/VK. Again we see that the VK result is in better agreement with the SCF and PDI results, and about 10% smaller than the SAOP/ALDA value. Both the SAOP/ALDA and the LDA/VK values are nonetheless well within the uncertainty range of 94 a.u. in the experimental result. The better agreement with the SCF result is, however, an indication that the LDA/VK result is more accurate, according to the rule of thumb that was found in the case of conjugated polymers [20,21].

In order to estimate the effect of going to very large tube lengths we also calculated the polarizability per

unit cell for a [5,5] carbon nanotube of infinite length. For the [5,5] carbon nanotube the unit cell consists of 20 carbon atoms. The calculations were done using the periodic structure version of the ADF program (BAND) [34], which uses the same methodology and basis-set types. We modified the TD-CDFT part [35] of this code to include the VK functional. Since the infinite [5,5] carbon nanotube has a semi-metallic band structure, we carefully checked that our results for the response calculations were converged with respect to the reciprocal space sampling. We used a valence triple zeta basis with two polarization functions, and a k-space sampling of 19 points in the one-dimensional irreducible wedge. As the SAOP is not available in the periodic structure code, we obtained the LDA/ALDA and LDA/VK results, and compare with the finite system results discussed above. Therefore we estimate the polarizability per unit cell,  $\Delta\alpha$  by calculating the difference in the polarizability of two successive fullerenes multiplied by two,  $\Delta\alpha(i) = 2(\alpha(C_{60+i \times 10}) - \alpha(C_{60+(i-1) \times 10}))$ , with  $i = 1-5$ . The results for  $\Delta\alpha_{\parallel}$  and the average value for  $\Delta\alpha_{\perp}$  are presented in Table 3 together with the values for the periodic structure calculations. The values for the polarizability per unit cell estimated from the finite fullerenes should extrapolate for large  $i$  to an asymptotic value in agreement with the results obtained for the infinite nanotube. For the perpendicular component that depends linearly on the size, we get an average value for  $\Delta\alpha_{\perp}$  of 152 a.u. using the LDA/VK results, which is about 10% smaller than the SAOP/ALDA result of 169 a.u. and which agrees quite well with the DPI model result of 142 a.u. The periodic structure calculation gives a similar reduction of 15%, from 150 a.u. (LDA/ALDA) to 128 a.u. (LDA/VK). For the parallel component of the polarizability per unit  $\Delta\alpha_{\parallel}$  we see a qualitatively different behavior, with the SAOP/ALDA result growing more steeply with system size than the LDA/VK results. The latter agree very well with the PDI model calculations. The SAOP/ALDA result is about 18% larger than the LDA/VK result for C<sub>60</sub>, which grows to 40% for C<sub>110</sub> and even 47% for the infinite nanotube result. These features are in accordance with the trends observed in the conjugated polymers [20,21].



Table 3

The SAOP/ALDA, LDA/VK, and PDI results for the polarizability (in a.u.) per unit cell,  $\Delta\alpha(i) = 2(\alpha(C_{60+i\times 10}) - \alpha(C_{60+(i-1)\times 10}))$ 

$i$	$\Delta\alpha_{\parallel}(i)$			$\Delta\bar{\alpha}_{\perp}$		
	SAOP/ALDA	LDA/VK	PDI	SAOP/ALDA	LDA/VK	PDI
1	354.6	299.7	282.1	—	—	—
2	376.8	306.6	290.6	—	—	—
3	425.4	337.5	326.9	—	—	—
4	520.6	376.5	—	—	—	—
5	555.8	397.0	351.3	168.7	151.8	141.6
$\infty$	(643.7)	438.4	—	(150.2)	128.3	—

The component parallel ( $\parallel$ ) to the long axis of the fullerenes is given as function of the number  $i$  of half unit cells, each containing 10 carbon atoms. The average for the perpendicular ( $\perp$ ) component is calculated using the first five values. The values with  $i = \infty$  correspond to the [5,5] carbon nanotube results. The LDA/ALDA result for the nanotube given in brackets can be used as estimate for the extrapolated SAOP/ALDA value.

In conclusion, we have presented accurate density functional response calculations for the static dipole–dipole polarizability of the tubular fullerenes  $C_{60+i\times 10}$  where  $i = 0–5$ , and for the closely related [5,5] nanotube. This was done by using a large basis set and both the conventional adiabatic local-density exchange–correlation functional and the more advanced Vignale–Kohn current-dependent functional describing long-range effects that cannot be included in the local-density functionals. The importance of the highly nonlocal exchange–correlation effects was exemplified by comparing the results for the fullerenes as function of the system size. For the  $C_{60}$  and  $C_{70}$  fullerenes, it was found that the current-functional results were in good agreement with experiment, and in much better agreement with available ab initio SCF results and model PDI results than the adiabatic local-density functional results. The excellent agreement with the model PDI results for the longer fullerenes suggests that the nonlocal xc-effects need to be included in the description of the polarizability. Large deviations in the longitudinal (perpendicular) polarizability per unit cell can otherwise be expected of up to 40–50% (10–15%) for the larger fullerenes and the [5,5] carbon nanotube.

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